

TOXICOKINETIC and/or UPTAKE MODELS (EIMS Version as of July 30, 2001)

For plant modeling, refer to the Runoff/Leaching and/or Water Distribution model survey form.

1) Model Acronym, Name, and Version:

Acronym and (name):

Version and (release date):

For abstract, see General Model Description

2) Overall Simulation and Linkage Capabilities of the Toxicokinetic and/or Uptake Model:

- ? Human and/or mammalian model
- ? Avian model
- ? Terrestrial invertebrates
- ? Aquatic vertebrate
- ? Aquatic invertebrates
- ? Simulates the effects of conventional chemical stressors on pollutant bio-uptake/toxicity
- ? Simulates the effects of non-chemical stressors on pollutant bio-uptake/toxicity
- ? Simulates the effects of mixture characteristics on individual pollutant bio-uptake/toxicity
- ? Mixture types
 - ? Chemical mixtures associated with manufacturing or processing
 - ? Chemical waste mixtures
 - ? Petroleum spills and/or wastes
 - ? Pesticide formulations
 - ? Other commercial/consumer chemical products (specify):
 - ? Other mixture types (specify):
- ? Monte Carlo/Latin Hypercube simulation
 - ? Internal Monte Carlo/Latin Hypercube software
 - ? Links to external Monte Carlo/Latin Hypercube software
 - ? Exportable to external Monte Carlo/Latin Hypercube Software
- ? Linked internally to an exposure model, sub-model, or module (specify):
- ? Linked externally to an exposure model, sub-model, or module (specify):
- ? Other simulation and/or linkage capabilities (specify):

3) Temporal Scale Options for the Overall Simulation:

- ? Hours
- ? Days
- ? Weeks
- ? Months
- ? One year

- ? Multiple years
- ? Other temporal scale options for the overall simulation (specify):

4) Type of, and Kinetic Resolution Scale of, the Toxicokinetic and/or Uptake Model:

- ? Empirically based one compartment (whole organism) model
- ? Empirically based two compartment model
- ? Empirically based multi-compartment model
- ? Physiologically based model with compartments representing physiological systems (e.g., respiratory, circulatory, upper digestive, excretory, endocrine, etc.)
- ? Physiologically based model with compartments representing individual organs and/or various sub-elements of differing resolution
 - ? Greatest kinetic resolution is at the whole organ level
 - ? Greatest kinetic resolution is at the organ component level (e.g., lung aveoli, gill lamella, intestinal villi, kidney tubulars)
 - ? Greatest kinetic resolution is at the cellular level
 - ? Greatest kinetic resolution is at the sub-cellular level (e.g., cell membranes, mitochondria)
 - ? Greatest kinetic resolution is at the molecular level
- ? Other type of, and/or kinetic resolution scale of, model (specify):

5) Governing Equations for the Toxicokinetic and/or Uptake Model:

- ? One pollutant mass balance ordinary differential equation (for a single compartment model) and its solution with the specified initial condition
- ? Two or more pollutant mass balance ordinary differential equations (for a multiple compartment model - one for each zone simulated) and their coupled solutions with the specified initial conditions
- ? Two or more pollutant continuity (mass balance) partial differential equations (for a multiple compartment model - one for each zone simulated) and their coupled solutions with the specified initial and boundary conditions
- ? Partial differential equations for pollutant diffusion within and across tissue and membranes
- ? Blood flow differential equations and their solutions
- ? Steady state solutions
- ? Transient solutions
- ? Analytical solutions
- ? Numerical solutions
- ? Other governing equations (specify):

6) Pollutant Intake Pathways for the Toxicokinetic and/or Uptake Model:

- ? Overall empirical intake rate
- ? Ingestion of food

- ? Ingestion of water
- ? Ingestion of soil, grit, or sediment
- ? Air inhalation
- ? Water ventilation over gills
- ? Dermal
- ? Other pollutant intake pathways (specify):

7) Pollutant Transport Processes for the Toxicokinetic and/or Uptake Model:

- ? Transport across dermal cells to interstitial fluid and/or to and across capillary walls
- ? Transport between interstitial fluid and blood across capillary walls
- ? Transport between interstitial fluid and tissue
- ? Respiratory system
 - ? Transport between air and aveoli capillaries
 - ? Transport between ventilation water and lamella capillaries
- ? Digestive system
 - ? Transport between intestinal fluids and villi capillaries
- ? Circulatory system
 - ? Lymphatic system (including transport between lymphatic and circulatory systems)
- ? Other pollutant transport processes (specify):

8) Pollutant Removal Pathways for the Toxicokinetic and/or Uptake Model:

- ? Overall empirical removal rate
- ? Filtering out of some particulate bound pollutants during respiration
- ? Air exhalation from the lungs or water removal from the gills
- ? Chemical transformations in the digestive tract
- ? Chemical transformations in the liver
- ? Renal filtration and urinary excretion
- ? Fecal excretion
- ? Perspiration excretion
- ? Other pollutant removal pathways (specify):

9) Temporal Resolution Options for the Output:

- ? Minutely
- ? Hourly
- ? Daily
- ? Weekly
- ? Monthly
- ? Annual
- ? Other temporal resolution options for the output (specify):

10) Input for the Toxicokinetic and/or Uptake Model:

- ? Refer to the abstract
- ? Refer to the user's manual (information for downloading and/or ordering is provided on the general model survey form)
- ? Individual input (**optional**): For input, referring to the abstract and/or the user's manual should be sufficient in most cases. However, as an option, additional information on individual input can be listed below:

11) Output of the Toxicokinetic and/or Uptake Model:

- ? Pollutant concentrations in the whole body as a function of time
- ? Pollutant concentrations in viscera (organs as a whole) as a function of time
- ? Pollutant concentrations in non-organ tissue as a function of time
- ? Pollutant concentrations in blood as a function of time
- ? Pollutant concentrations in interstitial fluid as a function of time
- ? Pollutant concentrations in excretion as a function of time
- ? Pollutant concentrations in exhaled air or water from the gills as a function of time
- ? Pollutant concentrations in individual organs as a function of time
- ? Pollutant concentrations in organ components as a function of time
- ? Pollutant concentrations in individual non-organ tissues (epidermal, connective, muscle, etc.) as a function of time
- ? Steady state, whole body BCFs for aquatic organisms
- ? Steady state pollutant concentrations in the whole body
- ? Steady state pollutant concentrations in viscera (organs as a whole)
- ? Steady state pollutant concentrations in non-organ tissue
- ? Steady state pollutant concentrations in blood
- ? Steady state pollutant concentrations in interstitial fluid
- ? Steady state pollutant concentrations in excretion
- ? Steady state pollutant concentrations in exhaled air or water from the gills
- ? Steady state pollutant concentrations in individual organs
- ? Steady state pollutant concentrations in organ components
- ? Steady state pollutant concentrations in individual non-organ tissues (epidermal, connective, muscle, etc.)
- ? Other significant output (specify):